International Journal of Chemical Studies

P-ISSN 2349–8528
E-ISSN 2321–4902
IJCS 2015; 2(5): 52-58

Received: 12-12-2014
Accepted: 15-01-2015

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Hyper-wiener index of gear fan and gear wheel related graph

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Abstract
The Hyper-Wiener index, as an extension of Wiener index, is an important topological index in Chemistry. There is a very close relation between the physical, chemical characteristics of many compounds and the topological structure of that. The Hyper-Wiener index is such a topological index and it has been widely used in Chemistry fields. In this paper, in terms of previous studies, we determine the Hyper-Wiener index of gear fan graph, gear wheel graph and their r-corona graphs.

Keywords: Chemical graph theory, organic molecules, Hyper-Wiener index, fan graph, wheel graph, gear fan graph, gear wheel graph, *r*-corona graph

1. Introduction

Chemical compounds and drugs are often modeled as graphs where each vertex represents an atom of molecule, and covalent bounds between atoms are represented by edges between the corresponding vertices. This graph derived from a chemical compounds is often called its molecular graph, and can be different structures. An indicator defined over this molecular graph, the Wiener index, has been shown to be strongly correlated to various chemical properties of the compounds. The Wiener index of a graph is defined as the sum of distances between all pairs of vertices of the graph. It has been found extensive applications in chemistry. Several years later, mathematician began to pay attention to the Wiener index and study it from the mathematical point of view. In such background, since each structural feature of organic molecule can be expressed as a graph, chemical graph theory as a branch of combinatorial chemistry is introduced to research the structure of molecule from graph theory standpoint.

The graphs considered in this paper are simple and connected. The vertex and edge sets of G are denoted by $V(G)$ and $E(G)$, respectively. The Wiener index is defined as the sum of distances between all unordered pair of vertices of a graph G, i.e.,

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v),$$

Where $d(u,v)$ is the distance between u and v in G.

Several papers contributed to determine the Wiener index of special graphs. Gao and Shi (Gao and Shi, in press) determined the Wiener index of gear fan graph, gear wheel graph and their *r*-corona graphs. Chen (Chen, 2005) [2] gained the exact expression for general pepoid graph. Xing and Cai (Xing and Cai, 2011) characterized the tree with third-minimum wiener index and introduce the method of obtaining the order of the Wiener indices among all the trees with given order and diameter, respectively. A tricyclic graph is a connected graph with n vertices and n+2 edges. Wan and Ren (Wan and Ren, 2012) [4] studied the Wiener index of tricyclic graph τ_n^3 which have at most a common vertex between any two circuits, and the smallest, the second-smallest Wiener indices of the tricyclic graphs τ_n^3 are given. The Hyper-Wiener index WW is one of the recently distance-based graph invariants. That WW clearly encodes the compactness of a structure and the WW of G is define as:

$$WW(G)=\frac{1}{2}\left(\sum_{\{u,v\}\subseteq V(G)} d(u,v)^2+\sum_{\{u,v\}\subseteq V(G)} d(u,v)\right)$$

Pan (Pan, 2013) deduced the formula of Wiener number and Hyper-Wiener number of two types of polyomino systems. More results on Wiener index and Hyper-Wiener index can refer to [6-13].

The graph $F_n=\{v\}\vee P_n$ is called a fan graph and the graph $W_n=\{v\}\vee C_n$ is called a wheel graph, where P_n is a path with n vertices and C_n is a cycle with n vertices. Graph $I_r(G)$ is called r- crown graph of G which splicing r hang edges for every vertex in G. The vertex set of hang edges that splicing of vertex v is called r-hang vertices, note v^*. By adding one vertex in every two adjacent vertices of the fan path P_n of fan graph F_n, the resulting graph is a subdivision graph called gear fan graph, denote as $\tilde{F}_n$. By adding one vertex in every two adjacent vertices of the wheel cycle C_n of wheel graph W_n, The resulting graph is a subdivision graph, called gear wheel graph, denoted as $\tilde{W}_n$.

In this paper, we present the Hyper-Wiener index of $I_r(F_n)$ and $I_r(W_n)$ first; then, the Hyper-Wiener index of gear fan graph and gear wheel graph are determined; at last, the Hyper-Wiener index of r-corona graph for $\tilde{F}_n$ and $\tilde{W}_n$ are derived.

2. Main results and proof

Theorem 1. $WW(I_r(F_n))=r^2(5n^2-\frac{3}{2}n+4)$.

$+r(\frac{3}{2}n^2+3n+2)+(6n^2-12n+\frac{9}{2})$

Proof. Let $P_n=v_1v_2\ldots v_n$ and the r hanging vertices of vi be v_i^1, v_i^2,…, v_i^r $(1\leq i\leq n)$. Let v be a vertex in F_n beside P_n, and the r hanging vertices of v be v^1, v^2, …, v^r.□

By the definition of Hyper-Wiener index, we have

$$WW(I_r(F_n))=\frac{1}{2}\{\{\sum_{i=1}^{r} d(v,v^i)+\sum_{i=1}^{n} d(v,v_i)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v,v_i^j)+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v^j)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r} d(v_i^j,v^k)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i,v_j)+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v_i^j)+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r} d(v_i,v_j^k)+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_i^j,v_i^k)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_i^k,v_j^t)\}$$

$$+\{\sum_{i=1}^{r} d(v,v^i)^2+\sum_{i=1}^{n} d(v,v_i)^2+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v,v_i^j)^2$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v^j)^2+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r} d(v_i^j,v^k)^2+$$

$$\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i,v_j)^2+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v_i^j)^2+$$

$$\sum_{i=1}^{n}\sum_{j\in\{1,\cdots,n\}-i}\sum_{k=1}^{r} d(v_i,v_j^k)^2+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_i^j,v_i^k)^2$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_i^k,v_j^t)^2\}\}$$

$$=\frac{1}{2}\{\{r+n+2nr+2nr+3nr^2+(n-1)^2+nr+r(3n^2-5n+2)$$

$$+nr(r-1)+r^2(n-1)(2n-1)\}+\{r+n+4nr+4nr+9nr^2+(2n^2-5n+3)+nr+(9n^2-19n+5)+2nr(r-1)+r^2(n-1)(8n-7)\}\}$$

$$=\frac{1}{2}\{\{r^2(2n^2+n+1)+r(3n^2-n+3)+(n^2-n+1)\}+\{r^2(8n^2-4n+7)+r(7n+1)+(11n^2-23n+8)\}\}$$

$$=r^2(5n^2-\frac{3}{2}n+4)+r(\frac{3}{2}n^2+3n+2)$$

$$+(6n^2-12n+\frac{9}{2}).$$

In this way, we get the decision. □

Theorem 2. $WW(I_r(W_n))=r^2(5n^2-\frac{3}{2}n)$

$+r(6n^2-\frac{13}{2}n+1)+(\frac{3}{2}n^2-\frac{5}{2}n)$.

Proof. Let $C_n=v_1v_2\ldots v_n$ and v_i^1, v_i^2,…, v_i^r be the r hanging vertices of vi $(1\leq i\leq n)$. Let v be a vertex in W_n beside C_n, and v^1, v^2, …, v^r be the r hanging vertices of v.

By the definition of Hyper-Wiener index, we have

$$WW(I_r(W_n))=\frac{1}{2}\{\{\sum_{i=1}^{r} d(v,v^i)+\sum_{i=1}^{n} d(v,v_i)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v,v_i^j)+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v^j)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r} d(v_i^j,v^k)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i,v_j)+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v_i^j)+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r} d(v_i,v_j^k)+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_i^j,v_i^k)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_i^k,v_j^t)\}$$

$$+\{\sum_{i=1}^{r} d(v,v^i)^2+\sum_{i=1}^{n} d(v,v_i)^2+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v,v_i^j)^2$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v^j)^2+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r} d(v_i^j,v^k)^2+$$

$$\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i,v_j)^2+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v_i^j)^2+$$

$$\sum_{i=1}^{n}\sum_{j\in\{1,\cdots,n\}-i}\sum_{k=1}^{r} d(v_i,v_j^k)^2+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_i^j,v_i^k)^2$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_i^k,v_j^t)^2\}\}$$

$$=\frac{1}{2}\{\{r+n+2nr+2nr+3nr^2+n(n-2)+nr+r(3n^2-5n)+nr(r-1)+r^2n(2n-3)\}+\{r+n+4nr+4nr+9nr^2+n(2n-5)+nr+r(9n^2-19n)+2nr(r-1)+r^2n(8n-15)\}\}$$

$$=\frac{1}{2}\{\{r^2(2n^2+n)+r(3n^2-n+1)+(n^2-n)\}+\{r^2(8n^2-4n)+r((9n^2-12n+1)+(2n^2-4n)\}\}$$

$$=r^2(5n^2-\frac{3}{2}n)+r(6n^2-\frac{13}{2}n+1)+(\frac{3}{2}n^2-\frac{5}{2}n)$$

Hence, we derive the desire conclusion. □

Taking r=0 in Theorem 1 and Theorem 2, we get following two corollaries.

Corollary 1. $WW(F_n)=6n^2-12n+\frac{9}{2}$

Corollary 2. $WW(W_n)=\frac{3}{2}n^2-\frac{5}{2}n$

Now, let us begin discussing the gear related graphs.

Theorem 3. $WW(\tilde{F}_n)=\frac{25}{2}n^2-\frac{71}{2}n+31$

Proof. Let $Pn=v1v2\ldots vn$ and $v_{i,i+1}$ be the adding vertex between vi and vi+1. Let v be a vertex in Fn beside Pn. By virtue of the definition of Hyper-Wiener index, we get

$$WW(\tilde{F}_n)=\frac{1}{2}\{\{\sum_{i=1}^{n} d(v,v_i)+\sum_{i=1}^{n-1} d(v,v_{i,i+1})+$$

$$\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i,v_j)+\sum_{i=1}^{n}\sum_{j=1}^{n-1} d(v_i,v_{j,j+1})$$

$$+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1} d(v_{i,i+1},v_{j,j+1})\}+\{\sum_{i=1}^{n} d(v,v_i)^2+$$

$$\sum_{i=1}^{n-1} d(v,v_{i,i+1})^2+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i,v_j)^2+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n-1} d(v_i,v_{j,j+1})^2+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1} d(v_{i,i+1},v_{j,j+1})^2\}\}$$

$$=\frac{1}{2}\{\{n+2(n-1)+n(n-1)+(3n^2-7n+4)+2(n-2)^2\}+\{n+4(n-1)+2n(n-1)+(9n^2-25n+16)+(8n^2-36n+40)\}\}$$

$$=\frac{1}{2}\{\{6n^2-13n+10\}+\{19n^2-58n+52\}\}$$

$$=\frac{25}{2}n^2-\frac{71}{2}n+31.$$

Thus, the desire result is given. □

Theorem 4. $WW(\tilde{W}_n)=\frac{25}{2}n^2-\frac{39}{2}n$

Proof. Let $C_n=v_1v_2\ldots v_n$ and v be a vertex in W_n beside C_n. Let $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1}. In view of the definition of Hyper-Wiener index, we deduce

$$WW(\tilde{W}_n)=\frac{1}{2}\{\{\sum_{i=1}^{n} d(v,v_i)+\sum_{i=1}^{n} d(v,v_{i,i+1})+$$

$$\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i,v_j)+\sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i,v_{j,j+1})$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_{i,i+1},v_{j,j+1})\}+\{\sum_{i=1}^{n} d(v,v_i)^2+$$

$$\sum_{i=1}^{n} d(v,v_{i,i+1})^2+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i,v_j)^2+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i,v_{j,j+1})^2+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_{i,i+1},v_{j,j+1})^2\}\}$$

$$= \frac{1}{2} \{\{n+2n+n(n-1)+(3n^2-4n)+n(2n-4)\}+\{n+4n+2n(n-1)+(9n^2-16n)+(8n^2-20n)\}\}$$

$$= \frac{1}{2}\{\{6n^2-6n\} + \{19n^2-33n\}\}$$

$$= \frac{25}{2}n^2 - \frac{39}{2}n.$$

Hence, we get the desire conclusion. $\square$

Theorem 5. $WW(I_r(\tilde{F}_n)) = (\frac{61}{2}n^2 - \frac{123}{2}n + \frac{99}{2})r^2 + (41n^2 - 100n + \frac{167}{2})r + (\frac{25}{2}n^2 - \frac{71}{2}n + 31)$.

Proof. Let $P_n=v_1v_2\ldots v_n$ and $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1}. Let v_i^1, v_i^2,…, v_i^r be the r hanging vertices of v_i $(1\le i\le n)$. Let $v_{i,i+1}^1$, $v_{i,i+1}^2$,…, $v_{i,i+1}^r$ be the r hanging vertices of $v_{i,i+1}$ $(1\le i\le n-1)$. Let v be a vertex in F_n beside P_n, and the r hanging vertices of v be v^1, v^2, …, v^r.

By virtue of the definition of Hyper-Wiener index, we get

$$WW(I_r(\tilde{F}_n)) = \frac{1}{2}\{\{\sum_{i=1}^{r} d(v,v^i) + \sum_{i=1}^{n} d(v,v_i)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v,v_i^j) + \sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v^j) +$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r} d(v_i^j,v^k) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i,v_j) +$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v_i^j) + \sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r} d(v_i,v_j^k) +$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_i^j,v_i^k) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_i^k,v_j^t)$$

$$+\sum_{i=1}^{n-1} d(v,v_{i,i+1}) + \sum_{i=1}^{n-1}\sum_{j=1}^{r} d(v,v_{i,i+1}^j)$$

$$+\sum_{i=1}^{r}\sum_{j=1}^{n-1} d(v^i,v_{j,j+1}) + \sum_{i=1}^{r}\sum_{j=1}^{n-1}\sum_{k=1}^{r} d(v^i,v_{j,j+1}^k) +$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n-1} d(v_i,v_{j,j+1}) + \sum_{i=1}^{n}\sum_{j=1}^{n-1}\sum_{k=1}^{r} d(v_i,v_{j,j+1}^k) +$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n-1} d(v_i^j,v_{k,k+1}) + \sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n-1}\sum_{t=1}^{r} d(v_i^j,v_{k,k+1}^t)$$

$$+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1} d(v_{i,i+1},v_{j,j+1}) + \sum_{i=1}^{n-1}\sum_{j=1}^{r} d(v_{i,i+1},v_{i,i+1}^j) +$$

$$\sum_{i=1}^{n-1}\sum_{j\in\{1,2,\cdots,n-1\}-i}\sum_{k=1}^{r} d(v_{i,i+1},v_{j,j+1}^k) +$$

$$\sum_{i=1}^{n-1}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_{i,i+1}^j,v_{i,i+1}^k) +$$

$$\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_{i,i+1}^k,v_{j,j+1}^t)\}+\{\sum_{i=1}^{r} d(v,v^i)^2 +$$

$$\sum_{i=1}^{n} d(v,v_i)^2 + \sum_{i=1}^{n}\sum_{j=1}^{r} d(v,v_i^j)^2 +$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v^j)^2 + \sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r} d(v_i^j,v^k)^2 +$$

$$\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i,v_j)^2 + \sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v_i^j)^2$$

$$+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r} d(v_i,v_j^k)^2 +$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_i^j,v_i^k)^2 + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_i^k,v_j^t)^2$$

$$+\sum_{i=1}^{n-1} d(v,v_{i,i+1})^2 + \sum_{i=1}^{n-1}\sum_{j=1}^{r} d(v,v_{i,i+1}^j)^2 +$$

$$\sum_{i=1}^{r}\sum_{j=1}^{n-1} d(v^i,v_{j,j+1})^2 + \sum_{i=1}^{r}\sum_{j=1}^{n-1}\sum_{k=1}^{r} d(v^i,v_{j,j+1}^k)^2$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n-1} d(v_i,v_{j,j+1})^2 + \sum_{i=1}^{n}\sum_{j=1}^{n-1}\sum_{k=1}^{r} d(v_i,v_{j,j+1}^k)^2$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n-1} d(v_i^j,v_{k,k+1})^2$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n-1}\sum_{t=1}^{r} d(v_i^j,v_{k,k+1}^t)^2 +$$

$$\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1} d(v_{i,i+1},v_{j,j+1})^2 + \sum_{i=1}^{n-1}\sum_{j=1}^{r} d(v_{i,i+1},v_{i,i+1}^j)^2$$

$$+\sum_{i=1}^{n-1}\sum_{j\in\{1,2,\cdots,n-1\}-i}\sum_{k=1}^{r} d(v_{i,i+1}, v^k_{j,j+1})^2 +$$

$$\sum_{i=1}^{n-1}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v^j_{i,i+1}, v^k_{i,i+1})^2 +$$

$$\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v^k_{i,i+1}, v^t_{j,j+1})^2 \}\}$$

$= \frac{1}{2}$ $\{\{r+n+2nr+2nr+3nr^2+n(n-1)+nr+3n(n-1)r+nr(r-1)+2r^2n(n-1)+2(n-1)+3r(n-1)+3r(n-1)+4r^2(n-1)+(n-1)(3n-4)+4r(n-1)^2+4r(n-1)^2+r^2(5n-4)(n-1)+2(n-2)^2+r(n-1)+r(5n^2-19n+18)+r(n-1)(r-1)+(n-2)(3n-5)r^2\}+\{r+n+4nr+4nr+9nr^2+2n(n-1)+nr+9n(n-1)r+2nr(r-1)+8r^2n(n-1)+4(n-1)+9r(n-1)+9r(n-1)+16r^2(n-1)+(n-1)(9n-16)+8(n-1)(2n-3)r+8(n-1)(2n-3)r+r^2(25n-32)(n-1)+4(n-2)(2n-5)+r(n-1)+r(25n^2-107n+114)+2r(n-1)(r-1)+(n-2)(18n-38)r^2\}\}$

$= \frac{1}{2}$ $\{\{r^2(10n^2-13n+9)+r(16n^2-28n+21)+(6n^2-13n+10)\}+\{r^2(51n^2-110n+90)+r(66n^2-172n+146)+(19n^2-58n+52)\}\}$

$$=(\frac{61}{2}n^2-\frac{123}{2}n+\frac{99}{2})r^2+(41n^2-100n+\frac{167}{2})r+(\frac{25}{2}n^2-\frac{71}{2}n+31)$$

Thus, the result is hold. □

Theorem 6. $WW(I_r(\tilde{W}_n))=(\frac{61}{2}n^2-\frac{53}{2}n)r^2+(41n^2-49n+1)r+(\frac{15}{2}n^2-\frac{39}{2}n)$.

Proof. Let $C_n=v_1v_2\ldots v_n$ and v be a vertex in W_n beside C_n. $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1}. Let v^1, v^2, …, v^r be the r hanging vertices of v and v_i^1, v_i^2, …, v_i^r be the r hanging vertices of v_i ($1\le i\le n$). Let $v_{n,n+1}=v_{1,n}$ and $v^1_{i,i+1}$, $v^2_{i,i+1}$, …, $v^r_{i,i+1}$ be the r hanging vertices of $v_{i,i+1}$ ($1\le i\le n$). In view of the definition of Hyper-Wiener index, we deduce

$$WW(I_r(\tilde{W}_n))=\frac{1}{2}\{\{\sum_{i=1}^{r}d(v,v^i)+\sum_{i=1}^{n}d(v,v_i)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v,v_i^j)+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i,v^j)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r}d(v_i^j,v^k)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}d(v_i,v_j)+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i,v_i^j)+\sum_{i=1}^{n}\sum_{j\in\{1,2,\cdots,n\}-i}\sum_{k=1}^{r}d(v_i,v_j^k)+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}d(v_i^j,v_i^k)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}d(v_i^k,v_j^t)$$

$$+\sum_{i=1}^{n}d(v,v_{i,i+1})+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v,v^j_{i,i+1})$$

$$+\sum_{i=1}^{r}\sum_{j=1}^{n}d(v^i,v_{j,j+1})+\sum_{i=1}^{r}\sum_{j=1}^{n}\sum_{k=1}^{r}d(v^i,v^k_{j,j+1})+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}d(v_i,v_{j,j+1})+\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r}d(v_i,v^k_{j,j+1})+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n}d(v_i^j,v_{k,k+1})+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n}\sum_{t=1}^{r}d(v_i^j,v^t_{k,k+1})$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}d(v_{i,i+1},v_{j,j+1})+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_{i,i+1},v^j_{i,i+1})+$$

$$\sum_{i=1}^{n}\sum_{j\in\{1,\cdots,n\}-i}\sum_{k=1}^{r}d(v_{i,i+1},v^k_{j,j+1})+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}d(v^j_{i,i+1},v^k_{i,i+1})$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}d(v^k_{i,i+1},v^t_{j,j+1})\}+\{\sum_{i=1}^{r}d(v,v^i)^2$$

$$+\sum_{i=1}^{n} d(v,v_i)^2 + \sum_{i=1}^{n}\sum_{j=1}^{r} d(v,v_i^j)^2$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v^j)^2 + \sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{r} d(v_i^j,v^k)^2 +$$

$$\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_i,v_j)^2 + \sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i,v_i^j)^2 +$$

$$\sum_{i=1}^{n}\sum_{j\in\{1,\cdots,n\}-i}\sum_{k=1}^{r} d(v_i,v_j^k)^2 + \sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_i^j,v_i^k)^2$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_i^k,v_j^t)^2 + \sum_{i=1}^{n} d(v,v_{i,i+1})^2 +$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r} d(v,v_{i,i+1}^j)^2 + \sum_{i=1}^{r}\sum_{j=1}^{n} d(v^i,v_{j,j+1})^2 +$$

$$\sum_{i=1}^{r}\sum_{j=1}^{n}\sum_{k=1}^{r} d(v^i,v_{j,j+1}^k)^2 + \sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i,v_{j,j+1})^2$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r} d(v_i,v_{j,j+1}^k)^2 + \sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n} d(v_i^j,v_{k,k+1})^2$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{k=1}^{n}\sum_{t=1}^{r} d(v_i^j,v_{k,k+1}^r)^2 +$$

$$\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_{i,i+1},v_{j,j+1})^2 + \sum_{i=1}^{n}\sum_{j=1}^{r} d(v_{i,i+1},v_{i,i+1}^j)^2 +$$

$$\sum_{i=1}^{n}\sum_{j\in\{1,\cdots,n\}-i}\sum_{k=1}^{r} d(v_{i,i+1},v_{j,j+1}^k)^2 + \sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_{i,i+1}^j,v_{i,i+1}^k)^2$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_{i,i+1}^k,v_{j,j+1}^t)^2 \}\}$$

$$= \frac{1}{2}\{\{r+n+2nr+2nr+3nr^2+n(n-1)+nr+3n(n-1)r+nr(r-1)+2n(n-1)r^2+2n+3rn+3rn+4r^2n+n(3n-4)+4rn(n-1)+4rn(n-1)+r^2n(5n-4)+2n(n-2)+rn+r(5n^2-9n)+nr(r-1)+(3n^2-5n)r^2\}+\{r+n+4nr+4nr+9nr^2+2n(n-1)+nr+9n(n-1)r+2nr(r-1)+8n(n-1)r^2+4n+9rn+9rn+16r^2n+(9n^2-16n)+r(16n^2-24n)+r(16n^2-24n)+r^2(25n^2-32n)+(8n^2-20n)+nr+r(25n^2-57n)+2nr(r-1)+(18n^2-38n)r^2\}\}$$

$$= \frac{1}{2}\{\{r^2(10n^2-4n)+r(16n^2-8n+1)+(6n^2-6n)\}+\{r^2(51n^2-49n)+r(66n^2-90n+1)+(19n^2-33n)\}\}$$

$$=(\frac{61}{2}n^2-\frac{53}{2}n)r^2+(41n^2-49n+1)r+(\frac{15}{2}n^2-\frac{39}{2}n)$$

As conclusion, we obtain the final conclusion.□

3. Conclusion

Combinatorial chemistry is a new powerful technology in molecular recognition and drug design. It is a wet-laboratory methodology purposed to massively parallel screening of chemical compounds for the founding of compounds that have certain biological activities. The power of trick draws from the interaction between computational modeling and experimental design.

Fan graph, wheel graph, gear fan graph, gear wheel graph and their *r*-corona graphs are common structural features of organic molecules. The contributions of our paper are determining the Hyper-Wiener index of these special structural features of organic molecules.

4. Acknowledgements

First, we thank the reviewers for their constructive comments in improving the quality of this paper. This work was supported in part by the PHD start funding of first author. We also would like to thank the anonymous referees for providing us with constructive comments and suggestions.

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